NASA TECHNICAL NOTE

NASA TN D-2170

NASA TN D-2170

DIRECT REACTION CALCULATION

by W. R. Gibbs, V. A. Madsen, J. A. Miller, W. Tobocman, E. C. Cox, and L. Mowry

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C. • FEBRUARY 1964

DIRECT REACTION CALCULATION

By

W. R. Gibbs
Los Alamos National Laboratory
Los Alamos, New Mexico

V. A. Madsen
Lewis Research Center
Cleveland, Ohio

J. A. Miller
Texaco Research Laboratory
Bellaire, Texas

W. Tobocman
Case Institute of Technology
Cleveland, Ohio

E. C. Cox
Lewis Research Center
Cleveland, Ohio

L. Mowry
I. B. M. Corporation (at Lewis)
Cleveland, Ohio

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

For sale by the Office of Technical Services, Department of Commerce,
Washington, D. C. 20230 -- Price $1.25

DIRECT REACTION CALCULATION

By W. R. Gibbs, V. A. Madsen, J. A. Miller,
W. Tobocman, E. C. Cox, and L. Mowry

Lewis Research Center

SUMMARY

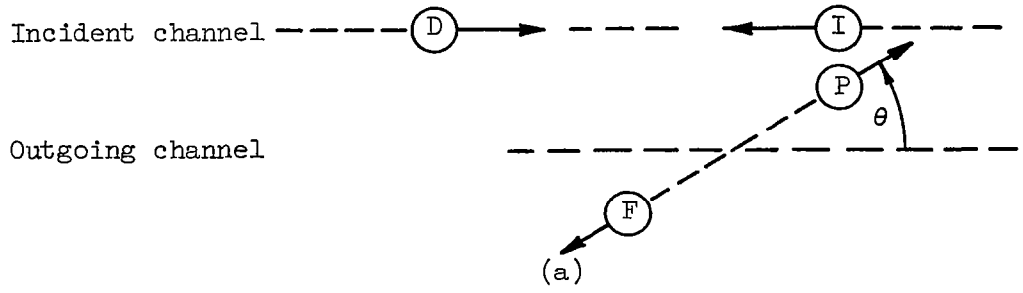
This report presents the program called DRC. It is an automatic computer program in the FORTRAN language for the calculation of transition amplitudes and cross sections on the basis of the distorted-wave Born approximation (DWBA). The incident- and the outgoing-channel wave functions used in the DWBA are descriptive of elastic scattering by an optical potential. DRC may be used to calculate the differential cross section for elastic scattering in both incident and outgoing channels. The following types of nuclear reactions can be treated by DRC: (1) inelastic scattering, (2) knock-out, (3) projectile stripping, and (4) target stripping.

INTRODUCTION

This report presents the program called DRC (direct reaction calculation). It is an automatic computer program in the FORTRAN language for the calculation of transition amplitudes and cross sections on the basis of the distorted-wave Born approximation (DWBA). The incident- and the outgoing-channel wave functions used in the DWBA are descriptive of elastic scattering by an optical potential. DRC may be used to calculate the differential cross section for elastic scattering in both incident and outgoing channels. The following types of nuclear reactions can be treated by DRC on the basis of the zero-range interaction approximation: (1) inelastic scattering, (2) knock-out, (3) projectile stripping, and (4) target stripping. For inelastic scattering there are two alternatives to the zero-range interaction approximation. The three inelastic scattering options are (1) single-particle excitation via a zero-range interaction, (2) single-particle excitation via a Yukawa interaction, and (3) collective excitation via a diffuse surface interaction.

BASIC MATHEMATICAL EQUATIONS

The DWBA formalism on which DRC is based will now be outlined. Let D be the incident particle, I the target nucleus, P the outgoing particle, and F the residual nucleus (sketch a).



According to the DWBA, the transition amplitude for this process is

$$A_{DP}(\vec{K}_D, \vec{K}_P) = \langle \Phi_{PF}^{(-)}(\vec{K}_P)\varphi_P\varphi_F | V_{PF} - \bar{V}_{PF} | \Phi_{DI}^{(+)}(\vec{K}_D)\varphi_D\varphi_I \rangle$$

where $\Phi_{AB}^{(\pm)}(\vec{K})$ is the wave function for the relative motion of particles A and B when the interaction between the two particles is the optical potential $\bar{V}_{AB}$ (ref. 1). When the superscript is +(-), the incoming (outgoing) part of $\Phi_{AB}(\vec{K})$ is asymptotically equal to the incoming (outgoing) part of $\exp i\vec{K} \cdot (\vec{r}_A - \vec{r}_B)$. When expanded in spherical harmonics,

$$\Phi_{AB}^{(+)}(\vec{K}) = 4\pi \sum_{l,m} i^l Y_l^m(\Omega_{\vec{K}})^* Y_l^m(\Omega_{\vec{r}}) f_l^{AB}(K, r)$$

where

$$\vec{r} = \vec{r}_A - \vec{r}_B$$

The equation for $\Phi^{(-)}$ is obtained by replacing f_l^{AB} by its complex conjugate. The wave function for the internal degrees of freedom of particle A is φ_A, while V_{PF} is the potential energy of interaction of particles P and F.

For inelastic scattering reactions P = D and F = I. When single-particle excitation is involved, I = C + N = F where C is the core and N is the bound particle. The transition amplitude is then

$$A_{DP}(\vec{K}_D, \vec{K}_P) = \sum (\lambda J_I \mu M_I | \lambda J_I J_F M_F) Q_\lambda^{l\bar{l}'jj'} F_{\lambda\mu}^{l\bar{l}'jj'}$$

where

$$F_{\lambda\mu}^{l\bar{l}'jj'} = \sum_{L,\bar{l}} \hat{\Gamma}_{L\bar{l}}^{\lambda\mu} F_\lambda^{l\bar{l}'jj'}(L\bar{l}) P_L^{|\mu|}(\cos\theta)$$

$$F_\lambda^{l\bar{l}'jj'}(L\bar{l}) = \int_0^\infty dr\, r^2 f_L^{PF}(K_P, r) f_l^{DI}(K_D, r) g_\lambda^{l\bar{l}'jj'}(r)$$

$$Q_\lambda^{l\bar{l}'jj'} = \sqrt{\frac{(2\lambda+1)(2\bar{l}+1)}{4\pi(2\bar{l}'+1)}} (\lambda\bar{l}00|\lambda l\bar{l}'0) \begin{Bmatrix} \lambda & j & j' \\ J_F & J_C & J_I \end{Bmatrix} \begin{Bmatrix} \lambda & \bar{l} & \bar{l}' \\ j' & J_N & j \end{Bmatrix}$$

$$\hat{\Gamma}_{L\bar{l}}^{\lambda\mu} = i^{l-L+\mu+|\mu|} \sqrt{4\pi(2\lambda+1)}\, \Gamma_{L\bar{l}}^{\lambda\mu}$$

$$\Gamma_{L\ell}^{\lambda\mu} = \frac{(2L+1)(2\ell+1)}{2\lambda+1}\sqrt{\frac{(L-\mu)!}{(L+\mu)!}}\,(L\ell\mu 0|\,L\ell\lambda\mu)(L\ell 00|\,L\ell\lambda 0)$$

$$\begin{Bmatrix} abc \\ def \end{Bmatrix} = -\sqrt{(2c+1)(2f+1)}\;W(abde;cf)$$

and where

$(j_1 j_2 m_1 m_2|\,j_1 j_2 JM)$ vector addition coefficient

$W(abde;cf)$ Racah coefficient

$P_\ell^m(x)$ associated Legendre polynomial

The form of $g_\lambda(r)$ depends on which option is chosen for the inelastic scattering interaction. If

$$V_{PF} - \overline{V}_{PF} = \frac{4\pi}{\alpha^3} V_0 \delta(\vec{r}_P - \vec{r}_N)$$

then

$$q_\lambda^{\ell\ell' jj'}(r) = \frac{4\pi V_0}{\alpha^3}\left(\frac{M_I}{M_C}\right)^3 \varphi_F^{\ell' j'}\left(\frac{M_I}{M_C}\,r\right)\varphi^{\ell j}\left(\frac{M_I}{M_C}\,r\right)$$

If

$$V_{PF} - \overline{V}_{PF} = \frac{V_0\, e^{-\alpha|\vec{r}_P - \vec{r}_N|}}{\alpha|\vec{r}_P - \vec{r}_N|}$$

then

$$g_\lambda^{\ell\ell' jj'}(r) = -4\pi V_0\left(\frac{M_I}{M_C}\right)^3 \int_0^\infty dr_1\, r_1^2 \varphi_F^{\ell' j'}\left(\frac{M_I}{M_C}\,r_1\right)\varphi_I^{\ell j}\left(\frac{M_I}{M_C}\,r_1\right) j_\lambda(i\alpha r_<)\, h_\lambda^{(1)}(i\alpha r_>)$$

where

$$\varphi_F^{J_F M_F} = \sum (J_I j M_I n|\,J_I j J_F M_F)(J_N \lambda M_N \mu|\,J_N l jn)\, Y_\lambda^\mu(\Omega)\,\varphi_N^{J_N M_N}\,\varphi_I^{J_I M_I}\,\varphi_F^{\lambda j}(r)$$

$$r_< = r \quad \text{if} \quad r < r_1$$

$$= r_1 \quad \text{if} \quad r_1 < r$$

and where

$j_\lambda(x)$ spherical Bessel function

$h_\lambda^{(1)}(x)$ spherical Hankel function of first kind

M_A mass of A

The expressions corresponding to inelastic scattering by collective excitation are similar to those given previously except that the superscripts $\overline{ll'}jj'$ are absent and the expressions for g_λ and Q_λ are modified. It is assumed that the incident particle D does not interact with a single particle N but instead interacts with a collective degree of freedom of the target nucleus I = F. Let

$$V_{PF} - \bar{V}_{PF} = \sum_{\lambda,\mu} \sqrt{\frac{4\pi}{2\lambda + 1}}\, v_\lambda(r_{PF}) Y_\lambda^\mu(\Omega_{PF})^* Y_\lambda^\mu(\Omega_F)$$

and use the relation

$$\langle \varphi_F | Y_\lambda^\mu(\Omega_F) | \varphi_I \rangle = \sqrt{\frac{(2\lambda + 1)(2J_I + 1)}{4\pi(2J_F + 1)}}\, (\lambda J_I \mu M | \lambda J_I J_F M_F)(\lambda J_I 0 M_I | \lambda J_I J_F M_F)$$

It follows that $g_\lambda = v_\lambda$. In this calculation

$$v_\lambda(r) = \frac{V_0 R_S}{a_S\left[2 + \exp\left(\frac{r - R_S}{a_S}\right) + \exp\left(\frac{R_S - r}{a_S}\right)\right]}$$

The amplitude for inelastic scattering by collective excitation then differs from that for single-particle excitation only in that $Q_\lambda^{\overline{ll'}jj'}$ is replaced by

$$Q_\lambda = \sqrt{\frac{2J_I + 1}{2J_F + 1}}\, (\lambda J_I 0 M_I | \lambda J_I J_F M_F)$$

In the previous discussion the contribution to inelastic scattering due to purely nuclear interactions was considered. There will also be a contribution arising from the Coulomb interaction. This may be introduced into the expressions by adding to the kernel g_λ a second term of the form

$$\hat{g}_\lambda(r) = \frac{4\pi}{2\lambda + 1}\left(\frac{M_I}{M_C}\right)^3 \int_0^\infty dr_1\, r_1^2 \rho_{FI}^\lambda\left(\frac{M_I}{M_C} r_1\right)\left[r_<^\lambda r_>^{-\lambda-1} - \delta_{\lambda 0} f(r)\right]$$

where

$$\rho_{FI}^{\lambda}(r) = \left[\int d\Omega \langle \varphi_F | \rho(\vec{r}) | \varphi_I \rangle Y_{\lambda}^{o}(\Omega) \right] \left(\frac{e\ Z_P}{4\pi\epsilon_o} \right)$$

$$f(r) = \begin{cases} 1/r & r > R_{NI} \\ 3/2\ R_{NI} - r^2/2\ R_{NI}^3 & r < R_{NI} \end{cases}$$

and $\rho(\vec{r})$ is the charge density operator. For single-particle excitation,

$$\rho_{FI}^{\lambda} = B_S \varphi_F^{\bar{l}' j'} \varphi_I^{lj} \frac{e^2 Z_P}{4\pi\epsilon_o}$$

For collective excitation,

$$\rho_{FI}^{\lambda} = B_S \frac{R_S}{a_S} \frac{\frac{e^2 Z_P Z_I}{4\pi\epsilon_o} \frac{3}{4\pi R_S^3}}{2 + \exp\left(\frac{r - R_S}{a_S} \right) + \exp\left(\frac{R_S - r}{a_S} \right)}$$

Finally, the program allows the nuclear collective interaction kernel to be given an alternative form to that of v_{λ}, namely,

$$g_{\lambda}(r) = -4\pi V_o \left(\frac{M_I}{M_C} \right)^3 \int_0^{\infty} dr_1\ r_1^2 j_{\lambda}(i\alpha r_<) h_{\lambda}^{(1)}(i\alpha r_>)$$

$$\times \frac{R_S}{a_S} \frac{\frac{3}{4\pi R_S^3}}{2 + \exp\left(\frac{\frac{M_I}{M_C} r - R_S}{a_S} \right) + \exp\left(\frac{R_S - \frac{M_I}{M_C} r}{a_S} \right)}$$

The cross section for inelastic scattering is

$$\sigma(\theta) = \frac{M_{PF}M_{DI}}{(2\pi\hbar^2)^2}\frac{K_P}{K_D}\frac{2J_F+1}{2J_I+1}\sum_{\lambda,\mu}\frac{\left|\sum_{\overline{ll'}jj'} Q_\lambda^{\overline{ll'}jj'} F_{\lambda\mu}^{\overline{ll'}jj'}\right|^2}{2\lambda+1}$$

for single-particle excitation and

$$\sigma(\theta) = \frac{M_{PF}M_{DI}}{(2\pi\hbar^2)^2}\frac{K_P}{K_D}\sum_{\lambda,\mu}\frac{(\lambda J_I 0 M_I | \lambda J_I 0 M_F | \lambda J_I J_F M_F)^2 |F_{\lambda\mu}|^2}{2\lambda+1}$$

for collective excitation. The reduced mass of A and B is M_{AB}. The DRC calculates the amplitude

$$B^{\lambda\mu} = i^{\mu+|\mu|+\lambda} F_{\lambda\mu}$$

and the cross section

$$\sigma(\theta) = \frac{M_{PF}M_{DI}}{(2\pi\hbar^2)^2}\frac{K_P}{K_D}\frac{2J_F+1}{2J_I+1}\sum_{\mu}\frac{|F_{\lambda\mu}|^2}{2\lambda+1}$$

The functions φ_I and φ_F used are normalized so that

$$1 = \int_0^\infty dr\, r^2\varphi(r)^2$$

Besides the DWBA amplitude and cross section described previously, the DRC calculates a second set of such quantities according to the cutoff DWBA. The cutoff DWBA differs from the DWBA only in that the kernel $g_{\lambda\mu}(r)$ is set equal to zero for r smaller than a cutoff radius R_C.

For knock-out reactions, $I = C + P$ and $F = C + D$, where C is the core. The interation $V_{PF} - \overline{V}_{PF} = V_{PD} + V_{PC} - \overline{V}_{PF}$ is approximated by $V_{PD} = (4\pi V_0/\alpha^3)\delta(\vec{r}_P - \vec{r}_D)$. The transition amplitude then becomes

$$A_{DP}(\vec{K}_D, \vec{K}_P) = \sum (ab\alpha\beta|ab\lambda\mu)(bJ_D\beta M_D|bJ_DJ_PM_P)(aJ_I\alpha M_I|aJ_IJ_FM_F) Q_{\lambda ab}^{\overline{ll}'jj'} F_{\lambda\mu}^{\overline{ll}'jj'}$$

where

$$F_{\lambda\mu}^{\overline{ll}'jj'} = \sum \hat{\Gamma}_{L\overline{l}}^{\lambda\mu} F^{\overline{ll}'jj'}(L\overline{l}) P_L^{|\mu|}(\cos\theta)$$

$$F^{\overline{ll}'jj'}(L\overline{l}) = \int_0^\infty dr\, r^2 f_L^{PF}\left(K_P, \frac{M_I}{M_F} r\right) f_{\overline{l}}^{DI}(K_D, r) g^{\overline{ll}'jj'}(r)$$

$$g^{\overline{ll}'jj'}(r) = \frac{4\pi V_0}{\alpha^3}\left(\frac{M_I}{M_C}\right)^3 \varphi_F^{l'j'}\left(\frac{M_I}{M_C} r\right) \varphi_I^{lj}\left(\frac{M_I}{M_C} r\right)$$

$$Q_{\lambda ab}^{\overline{ll}'jj'} = \sum_c (-1)^{J_C - J_F - J_P + j - j' + \overline{l} - \overline{l}' + b - c} (\lambda\overline{l}00|\lambda\overline{ll}'0) \begin{Bmatrix} J_D & \overline{l}' & j' \\ J_P & c & b \end{Bmatrix}$$

$$\times \sqrt{\frac{(2b+1)(2c+1)(2\overline{l}+1)(2J_I+1)}{4\pi(2l'+1)(2J_C+1)(2J_P+1)}} \begin{Bmatrix} \lambda & \overline{l} & \overline{l}' \\ b & c & a \end{Bmatrix} \begin{Bmatrix} J_I & j & J_C \\ J_F & j' & a \end{Bmatrix} \begin{Bmatrix} J_P & \overline{l} & j \\ j' & a & c \end{Bmatrix}$$

The cross section is

$$\sigma(\theta) = \frac{M_{ID}M_{FP}}{(2\pi\hbar^2)^2} \frac{K_P}{K} \frac{(2J_P+1)(2J_F+1)}{(2J_D+1)(2J_I+1)} \sum_{\lambda\mu ab} \frac{\left| \sum_{\overline{ll}'jj'} F_{\lambda\mu}^{\overline{ll}'jj'} Q_{\lambda ab}^{\overline{ll}'jj'} \right|^2}{(2a+1)(2b+1)}$$

The DRC calculates the amplitude

$$B^{\lambda\mu} = i^{\mu + |\mu| + \lambda} F_{\lambda\mu}^{\overline{ll}'jj'}$$

and the cross section

$$\sigma(\theta) = \frac{M_{ID}M_{FP}}{(2\pi\hbar^2)^2}\frac{K_P}{K_D}\frac{(2J_P+1)(2J_F+1)}{(2J_D+1)(2J_I+1)}\sum_{\mu}\left|F_{\lambda\mu}^{ll'jj'}\right|^2$$

For projectile stripping reactions $D = N + P$ and $F = I + N$, where N is the exchanged particle. The interaction $V_{PF} - \bar{V}_{PF} = V_{PN} + V_{PI} - \bar{V}_{PF}$ is approximated by V_{PN}. The interaction V_{PN} is taken to have zero range so that

$$V_{PN}\varphi_D = -\sqrt{8\pi E_B^{1/2}\left(\frac{\hbar^2}{2M_{PN}}\right)^{3/2}}\,\delta(\vec{r}_N - \vec{r}_P)$$

$$= -W_{NP}\delta(\vec{r}_N - \vec{r}_P)$$

where E_B is the binding energy of D. The transition amplitude then becomes

$$A_{DP}(\vec{K}_D,\vec{K}_P) = \sum (J_I jM_I n|J_I jJ_F M_F)(J_N\lambda M_N\mu|J_N\lambda jn)(J_P J_N M_P M_N|J_P J_N J_D M_D)F_{\lambda\mu}^{j}$$

where

$$F_{\lambda\mu}^{j} = \sum \hat{\Gamma}_{Ll}^{\lambda\mu}F_{\lambda}^{j}(Ll)P_L^{|\mu|}(\cos\theta)$$

$$F_{\lambda}^{j}(Ll) = \int_0^{\infty} dr\, r^2\, f_L^{PF}\left(K_P, \frac{M_I}{M_F}r\right) f_l^{DI}(K_D, r)g_{\lambda}^{j}(r)$$

$$g_{\lambda}^{j}(r) = -W_{NP}\varphi_F^{\lambda j}(r)$$

The cross section is

$$\sigma(\theta) = \frac{M_{DI}M_{PF}}{(2\pi\hbar^2)^2}\frac{K_P}{K_D}\frac{2J_F+1}{(2J_I+1)(2J_N+1)}\sum_{j\lambda\mu}\frac{\left|F_{\lambda\mu}^{j}\right|^2}{2\lambda+1}$$

The DRC calculates the amplitude

$$B^{\lambda\mu} = i^{\mu+|\mu|+\lambda}F_{\lambda\mu}^{j}$$

and the cross section

$$\sigma(\theta) = \frac{M_{DI} M_{PF}}{(2\pi\hbar^2)^2} \frac{K_P}{K_D} \frac{2J_F + 1}{(2J_I + 1)(2J_N + 1)} \sum_{\mu} \frac{\left| F^j_{\lambda\mu} \right|^2}{2\lambda + 1}$$

For target stripping reactions I identifies the incident projectile and D = P + N identifies the target nucleus. The residual nucleus is F = I + N and the outcoming particle is P. The expressions for the transition amplitude and cross section are then identical to those for projectile stripping except that $\vec{K}_D$ must be replaced by $-\vec{K}_I$. Thus,

$$A_{IP}(K_I, K_P)_t = A_{DP}(-K_D, K_P)_p$$

and

$$\sigma(\theta)_t = \sigma(\pi - \theta)_p$$

where the subscripts t and p denote target and projectile stripping, respectively. The DRC uses these relations to calculate the transition amplitude $B^{\lambda\mu}$ and differential cross section $\sigma(\theta)$ for target stripping from the corresponding quantities for projectile stripping.

The DRC consists of a set of subprograms that run sequentially. These programs make use of a group of subroutines and function subprograms. For convenience in compilation, the subprograms are arranged into four subsets called links.

LIST OF SUBPROGRAMS

Main Program

Link 1

0	Input data reduction
IZS	Surface-interaction form factor
IZA	Bound-state wave functions
IZB	Bound-states multiplication
IZC	Bound-states kernel

Link 2

2VD	Kinetic energy for incident channel
2VP	Kinetic energy for outgoing channel

	2XD	Radial wave function for incident channel
	2XP	Radial wave function for outgoing channel
Link 3		
	3B	Coulomb scattering amplitudes
	3A	Nuclear scattering amplitudes
	4	Radial integrals
	5	Coefficients of Legendre polynomial expansion
Link 4		
	6	Convergence test and total cross section
	7A	Direct-reaction amplitudes
	7B	Direct-reaction cross sections
	8	Elastic scattering cross sections

Subroutines and Function Subprograms

SZ	Surface form factor
AJH	Spherical Bessel or Hankel function
ONE Z	Bound-state wave function
TWO PD	Kinetic energy (Saxon well + Coulomb well)
TWO AB	Radial wave function
THREE A	Nuclear scattering amplitudes
THREE B	Coulomb scattering amplitude
FOUR	Radial integral
LP	Associated Legendre polynomials
GAMMA	Gamma coefficient
FCTRL	Factorial function
PLOT	Plot graph
PLOTMY	Plot graph II

VBEST Harmonic oscillator potential depth

INTRP Interpolation

INPUT DECK

The information to be entered on each card of the input deck and the format to be used are given by the following list:

(1) Information to identify calculation (80H)

(2)	IREACH	LIL	LPAR	NOLD	IPPAR	IWRTZ (6I4)
(3)	ZI	ZF	ZD	ZP		(1P4E 15.8)
(4)	JI	JF	JD	JP		(1P4E 15.8)
(5)	MI	MF	MD	MP		(1P4E 15.8)
(6)	ZN	JN	MN	YS		(1P4E 15.8)
(7)	L1	L2	N1	N2		(1P4E 15.8)
(8)	ED	Q	EB	QB		(1P4E 15.8)
(9)	LAM	RC	R2	M		(1P4E 15.8)
(10)	VD	WD	RD	AD		(1P4E 15.8)
(11)	XD	XRD	XAD	YL		(1P4E 15.8)
(12)	VP	WP	RP	AP		(1P4E 15.8)
(13)	XP	XRP	XAP	BS		(1P4E 15.8)
(14)	RS	AS	VO	ALPHA		(1P4E 15.8)
(15)	VN1	RN1	BN1	CS1		(1P4E 15.8)
(16)	VN2	RN2	BN2	CS2		(1P4E 15.8)
(17)	AJ1	AJ2	DVN	AN3		(1P4E 15.8)
(18)	DELTAO	AN0	AN2	AN5		(1P4E 15.8)
(19)	AN6	AN8	AN9	AN10		(1P4E 15.8)
(20)	W1	W2	W3	W4		(1P4E 15.8)
(21-1)	XST	THETAO	DELTA	NOT		(3E 15.8, I 10)
	.	.	.	.	.	.
	.	.	.	.	.	.
	.	.	.	.	.	.
(21-NOT)	XST	THETAO	DELTA	NOT		(3E 15.8, I 10)

(22) Information to identify plot (12 A6)

(23) NE THETE DELTE (I5, 2E 15.8)

If LPAR $\neq$ 0 or if AN5 $\neq$ 0, card 23 should be left out.

The quantities just listed are to be interpreted as follows:

IREACN = I_R determines type of reaction to be calculated

I_R = 1 inelastic scattering

I_R = 2 knock-out

= 3 projectile stripping

= 4 target stripping

LIL = L_I determines form of interaction

L_I = 0 surface interaction

= 1 Yukawa well interaction

= 2 zero-range interaction

= 3 Yukawa well-surface interaction

LPAR = L_P allows continuum wave function part of calculation to be omitted

L_P = 0 calculation proceeds in usual way

= 1 program does not calculate continuum radial wave functions but uses instead those written on tape by a previous calculation

NOLD = N_D determines type of potential well used to calculate bound-state wave functions

N_D = 1 Saxon well

= 2 truncated harmonic oscillator well

= 3 harmonic oscillator well

IPPAR = I_P allows transition amplitudes to be read out

I_P = 0 transition amplitudes are printed out

> 0 transition amplitudes are printed out and punched out on cards

< 0 transition amplitudes are not read out

IWRTZ = I_{WZ} if $I_{WZ} \neq 0$ bound-state wave functions and potential form factors are printed out

ZI = Z_I charge of target nucleus

ZF = Z_F charge of residual nucleus

ZD = Z_D charge of incident particle

ZP = Z_P charge of outgoing particle

JI = J_I spin of target nucleus

JF = J_F spin of residual nucleus

JD = J_D spin of incident particle

JP = J_P spin of outgoing particle

MI = M_I mass of target nucleus

MF = M_F mass of residual particle

MD = M_D mass of incident particle

MP = M_P mass of outgoing particle

If $I_R = 4$, then I identifies incident particle and D identifies target nucleus instead of what is shown previously.

ZN = Z_N charge of bound particle

JN = J_N spin of bound particle

MN = M_N mass of bound particle

YS = Y_S determines verticle scale of graphical output

L1 = $\overline{l}$ orbital angular momentum of particle bound in target nucleus

L2 = $\overline{l}'$ orbital angular momentum of particle bound in residual nucleus

N1 = $\overline{n}$ radial quantum number of particle in target nucleus, number of nodes of radial wave function plus one

N2 = $\overline{n}'$ radial quantum number of particle in residual nucleus

ED = E_D laboratory energy of incident particle

Q = Q Q-value of reaction, positive for exothermic reactions

EB = E_B — binding energy of target nucleus or incident particle, separation energy

QB = Q_B — binding energy of residual nucleus minus E_B

LAM = λ — angular momenum transfer

RC = R_C — cutoff radius

R2 = R_2 — interval doubling radius; R_2 should be set so that it is about equal to R_{N1} and R_{N2}

M = m — Saxon well flattening parameter

VD = V_D — depth of real part of optical potential for incident channel, negative channel, negative for attractive potential

WD = W_D — depth of imaginary part of optical potential for incident channel, negative for absorptive potential

RD = R_D — radius of Saxon well for incident channel

AD = a_D — diffuseness of optical potential for incident channel

XD = X_D — strength of surface absorption potential for incident channel, negative for absorptive potential

XRD = XR_D — radius of surface absorption potential for incident channel

XAD = Xa_D — diffuseness of surface absorption potential for incident channel

YL = Y_L — determines whether cross section ($Y_L = 0$) or logarithm of the cross section ($Y_L \neq 0$) appears in graphical output

VP = V_P — depth of real part of optical potential for outgoing channel, negative for attractive potential

WP = W_P — depth of imaginary part of optical potential for outgoing channel, negative for absorptive potential

RP = R_P — radius of Saxon well for outgoing channel

AP = a_P — diffuseness of optical potential for outgoing channel

XP = X_P — strength of surface absorption potential for outgoing channel, negative for absorptive potential

XRP = XR_P — radius of surface absorption potential for outgoing channel

XAP = Xa_P — diffuseness of surface absorption potential for outgoing channel

BS = B_S	strength of Coulomb interaction
RS = R_S	radius of surface-interaction form factor
AS = a_S	diffuseness of surface-interaction form factor
VO = V_O	strength of inelastic scattering interaction, negative for attractive interaction
ALPHA = α	range of inelastic scattering interaction
VNI = V_{NI}	depth estimate of potential well for initial bound state, positive for attractive potential
RN1 = R_{N1}	radius of potential well for initial bound state
BN1 = B_{N1}	shape parameter for potential well for initial bound state
CS1 = C_{S1}	spin-orbit parameter for potential well for initial bound state
VN2 = V_{N2}	depth estimate of potential well for final bound state
RN2 = R_{N2}	radius of potential well for final bound state
BN2 = B_{N2}	shape parameter for potential well for final bound state
CS2 = C_{S2}	spin-orbit parameter for potential well for final bound state
AJ1 = j_1	total angular momentum of initial bound particle
AJ2 = j_2	total angular momentum of final bound particle
DVN = D_{VN}	increment in potential depth used in search for correct bound-state potential well depth
AN3 = N_3	convergence criterion used in well-depth search
DELTAO = δ_O	mesh interval size
ANO = N_O	determines transition point in radial wave-function calculation
AN2 = N_2	convergence criterion for asymptotic series used in radial wave-function calculation
AN5 = N_5	elastic cross sections will not be read out if $N_5 \neq 0$
AN6 = N_6	convergence criterion for power series used in radial wave-function calculation
AN8 = N_8	criterion for setting upper limit for radial integrals

AN9 = N_9 criterion for setting Saxon form factor equal to zero

AN10 = N_{10} maximum number of terms to be allowed in asymptotic series

W1 = W_1 criterion for determining number of partial waves to be distorted in incident channel

W2 = W_2 criterion for determining number of partial waves to be distorted in outgoing channel

W3 = W_3 allows bound-state kernel part of calculation to be omitted

$W_3 = 0$ calculation proceeds in usual way

$W_3 \neq 0$ calculation of bound-state kernel in link 1 is omitted, kernel is placed in memory by previous calculation used

W4 = W_4 criterion for determining total number of partial waves used

XST = σ_{EX} experimental differential cross section

THETA0 = θ DELTA = Δ NOT = N_T

If $\Delta = 0$, there should be N_T cards bearing numbers identified by σ_{EX}, θ, Δ, and N_T. The quantities Δ and N_T need be present only on the first of this group of cards. The quantities σ_{EX} and θ will be different on each card. They will represent the observed differential cross section and the center of mass angle at which it is observed. The program will calculate a theoretical differential cross section at each of these angles. If $\Delta \neq 0$, there should be only one card bearing numbers identified by σ_{EX}, θ, Δ, and N_T. In this case σ_{EX} is ignored, and the program calculates the direct-reaction differential cross section at the center of mass angles θ, $\theta + \Delta$, $\theta + 2\Delta$, . . ., $\theta + (N_T - 1)\Delta$:

NE = N_E THETE = θ_E DELTE = Δ_E

The elastic differential cross sections will be calculated at the center of mass angles θ_E, $\theta_E + \Delta_E$, $\theta_E + 2\Delta_E$, . . ., $\theta_E + (N_E - 1)\Delta_E$. There should be no more than 100 points in any of these angular distributions. The input information should be in the following units:

angle	degrees
angular momentum	units of $\hbar$
charge	units of charge of the positron
differential cross section	millibarns per steradian
energy	million electron volts (Mev)

length fermis

mass atomic mass units

DESCRIPTION OF SUBPROGRAMS

Program 0 - Input Data Reduction

Program 0 reads part of the input information and prepares it for use in subsequent parts of the calculation.

The first card of the input deck contains whatever information it is desired to use to identify the calculation. The contents of the first 20 input cards are printed out to help identify the output. The contents of input cards 2 to 19 appear under the heading INPUT TO PART ZERO. Then under the heading OUTPUT FROM PART ZERO the following numbers are printed out:

ED = E_D

KD = $K_D = (2M_{ID}^2 E_D / M_D \hbar^2)^{1/2}$

AETAD = $\eta_D = Z_D Z_I M_{ID} c / K_D \hat{\alpha} \hbar$

MID = $M_{ID} = M_I M_D / (M_I + M_D)$

EP = $E_P = [M_I E_D + (M_I + M_D)Q] / M_F$

KP = $K_P = (2M_{FP}^2 E_P / M_P \hbar^2)^{1/2}$

AETAP = $\eta_P = Z_P Z_F M_{FP} c / K_P \hat{\alpha} \hbar$

MFP = $M_{FP} = M_F M_P / (M_F + M_P)$

EN1 = $E_{N1} = E_B$

KN1 = $K_{N1} = (2M_{NC} E_B / \hbar^2)^{1/2}$ $\quad I_R = 1, 2$

$= 0$ $\quad I_R = 3, 4$

AETANI = $\eta_{NI} = Z_N (Z_I - Z_N) M_{NC} c / K_{NI} \hat{\alpha} \hbar$ $\quad I_R = 1, 2$

$= 0$ $\quad I_R = 3, 4$

$M1 = M_1 = M_N(M_I - M_N)/M_I = M_{NC}$

$EN2 = E_{N2} = E_B + Q_B$

$KN2 = K_{N2} = (2M_2E_{N2}/\hbar^2)^{1/2}$

$AETAN2 = \eta_{N2} = Z_N(Z_I - Z_N)M_2c/K_{N2}\hat{\alpha}\hbar \qquad I_R = 1$

$= Z_D(Z_I - Z_N)M_2c/K_{N2}\hat{\alpha}\hbar \qquad I_R = 2$

$= Z_NZ_IM_2c/K_{N2}\hat{\alpha}\hbar \qquad I_R = 3,4$

$M2 = M_2 = M_N(M_I - M_N)/M_I \qquad I_R = 1$

$= M_D(M_F - M_D)/M_F \qquad I_R = 2$

$= M_IM_N/M_F \qquad I_R = 3,4$

$AEPS = \epsilon = \delta_O/(K_P + K_D)$

$AEPN = \epsilon_N = \epsilon M_I/(M_I - M_N) \qquad I_R = 1,2$

$= \epsilon M_F/M_I \qquad I_R = 3,4$

$AEPD = \epsilon_D = \epsilon \qquad I_R = 1,2$

$= \epsilon M_F/M_I \qquad I_R = 3,4$

$AEPP = \epsilon_P = \epsilon \qquad I_R = 1,3,4$

$= \epsilon M_I/M_F \qquad I_R = 2$

$RO = R_O \approx R_{N2} - 2\epsilon_N + N_8/(K_{N1} + K_{N2}) \qquad L_I = 1,2$

$\approx R_S - 2\epsilon_N + N_8a_S \qquad L = 0,3$

$RC = R_C \approx R_C$

$R2 = R_2 \approx R_2$

$AIPE = P = 1 + e^{-m}$

$$\text{RDB} = \bar{R}_D = R_D - a_D \ln(1 + 2e^{-m})$$

$$\text{RPB} = \bar{R}_P = R_P - a_P \ln(1 + 2e^{-m})$$

$$\text{ROD} = \rho_D = \bar{R}_D - ma_D$$

$$\text{ROP} = \rho_P = \bar{R}_P - ma_P$$

$$\text{SD} = S_D = \text{Max}[S_D^{(1)}, S_D^{(2)}]$$

$$S_D^{(1)} = \bar{R}_D + a_D(0.69315 + 2.302585\ N_9)$$

$$S_D^{(2)} = XR_D + Xa_D(0.69315 + 2.302585\ N_9)$$

$$\text{SP} = S_P = \text{Max}[S_P^{(1)}, S_P^{(2)}]$$

$$S_P^{(1)} = \bar{R}_P + a_P(0.69315 + 2.302585\ N_9)$$

$$S_P^{(2)} = XR_P + Xa_P(0.69315 + 2.302585\ N_9)$$

$$\text{COD} = C_{OD} = \left\{2\pi\eta_D/[\exp(2\pi\eta_D) - 1]\right\}^{1/2}$$

$$\text{COP} = C_{OP} = \left\{2\pi\eta_P/[\exp(2\pi\eta_P) - 1]\right\}^{1/2}$$

$$\text{VI} = V_I = [4\pi(2\lambda + 1)]^{1/2}/K_P K_D \qquad I_R = 1,\ L_I = 0$$

$$= 1.5[4\pi(2\lambda + 1)]^{1/2}/K_P K_D \qquad I_R = 1,\ L_I = 1$$

$$= (4\pi)^{3/2}(2\lambda + 1)^{1/2}\ V_0 M_I^3/K_P K_D \alpha^3 M_C^3 \qquad I_R = 1,\ L_I = 2$$

$$= (4\pi)^{3/2}(2\lambda + 1)^{1/2}\ V_0 M_I^2 M_F/K_P K_D \alpha^3 M_C^3 \qquad I_R = 2$$

$$= -[32\pi(2\lambda + 1)E_B^{1/2}/K_P K_D]^{1/2}(M_F^2/M_I^2)$$

$$\times [\hbar^2(M_N + M_P)/2M_N M_P]^{3/4} \qquad I_R = 3, 4$$

$$\text{AETA} = \eta = \eta_0(2\lambda + 1)^{-1} \qquad I_R = 1$$

$$= \eta_0(2J_P + 1)/(2J_D + 1) \qquad I_R = 2$$

$$= \eta_0(2\lambda + 1)^{-1}(2J_N + 1)^{-1} \qquad I_R = 3, 4$$

$$\eta_0 = 10\, M_{ID} M_{FP} (2\pi\hbar^2)^{-2} K_P K_D^{-1} (2J_F + 1)(2J_I + 1)^{-1}$$

$$\text{MC} = M_C = M_I - M_N \qquad I_R = 1$$

$$= M_F - M_D \qquad I_R = 2$$

$$= M_F - M_N \qquad I_R = 3, 4$$

$$\text{NR2} = n_2 = R_2/\epsilon_N$$

$$\text{NRO} = n_0 = (R_2/\epsilon_N) + (R_0 - R_2)/2\epsilon_N$$

$$\text{NRC} = n_C = (R_C/\epsilon_N) + (R_C - R_2 + |R_C - R_2|)/4\epsilon_N$$

$$\text{LAM} = \lambda$$

$$\text{LDD} = L_{DD} = K_D R_D + W_1$$

$$\text{LDP} = L_{DP} = K_P R_P + W_2$$

$$\text{LCD} = L_{CD} = L_{CP} + \lambda$$

$$\text{LCP} = L_{CP} = \text{MAX}(L_{DD}, L_{DP}, K_P R_0 + W_4)$$

where

$\hbar^2 = 41.826134$

$\hat{\alpha}^{-1} = 7.2973254 \times 10^{-3}$

$c/\hbar = 4.7195563$

Limitations inherent in the program impose certain restrictions on some of these numbers. It is necessary that n_0 be less than 500. If n_0 is greater than 499, NO TOO LARGE is printed out, n_0 is set equal to 499, and the calculation continues. It is also necessary that L_{DD}, L_{DP}, L_{CD}, and L_{CP} each be less

than 50 and λ be less than 6. Also, it is necessary that $L_{DD} < L_{CD}$ and $L_{DP} < L_{CP}$.

Program IZS - Surface-Interaction Form Factor

If $L_I \neq 0,3$, program IZS is skipped and control is shifted to program IZA. Program IZS calls subroutine SZ to calculate the function

$$ZDEL(n) = R_S V_0 a_S^{-1} \left[2 + \exp\left(\frac{r - R_S}{a_S}\right) + \exp\left(\frac{R_S - r}{a_S}\right) \right]^{-1}$$

where

$$r = n\epsilon_N \qquad n \leq n_2$$

$$= R_2 + (n - n_2)2\epsilon_N \qquad n > n_2$$

which will be used as the bound-state kernel in program 4. After ZDEL is calculated in this manner, control is shifted to program 2VD.

The description of IZS applies only if $L_I \neq 3$ and $B_S = 0$. If $L_I = 0$ and $B_S \neq 0$, the program calculates ZDEL as just described and in addition calculates

$$ZC = R_S a_S^{-1} \left[2 + \exp\left(\frac{r - R_S}{a_S}\right) + \exp\left(\frac{R_S - r}{a_S}\right) \right]^{-1}$$

and shifts control to the middle of program IZB. If $L_I = 3$, ZDEL is not calculated, ZC is calculated as described, and control is shifted to the middle of program IZB. When $L_I = 0$, IZB and IZC will add a Coulomb term to the kernel ZDEL. When $L_I = 3$, IZB and IZC will calculate both the nuclear and the Coulomb contributions to the kernel.

Program IZA - Bound-State Wave Functions

Program IZA uses subroutine ONE Z to calculate the radial wave functions of the bound particles. If $L_I = 1$, the bound-state wave functions are calculated with a mesh size of $\frac{1}{3}\epsilon_N$ instead of ϵ_N so that they may be folded together with the spherical Bessel functions in program IZC. If $I_R = 1$ or 2, the program calculates two bound-state wave functions: AZ(n) with parameters $\bar{l}$, η_{NI}, $\bar{n}$, and K_{N1} and ZB(n) with parameters $\bar{l}'$, η_{N2}, $\bar{n}'$, and K_{N2}. If $I_R = 3$ or 4, the program only calculates ZB(n).

Program IZB - Bound-State Multiplication

If $I_R = 3$ or 4 and $L_I \neq 0,3$, the function ZDEL(n) is set equal to ZB(n); if $I_R = 1$ or 2 and $L_I = 2$, then ZDEL(n) is set equal to ZA(n) · ZB(n); if $I_R = 1$ and $L_I = 1$, then ZC = ZA · ZB; and if $I_R = 1$ and $L_I = 3$, then ZC is provided by program IZS. These ZC's are used to calculate the nuclear kernel. If $I_R = 1$ and $B_S \neq 0$, then a ZC will be provided for the calculation of the Coulomb kernel for all four values of L_I.

When the nuclear kernel is being calculated, IZB computes

$$ZA1(n) = ZC(n)j_\lambda(i\alpha r) \quad \begin{matrix} 1 & \text{even } \lambda \\ 1 & \text{odd } \lambda \end{matrix}$$

$$ZA2(n) = ZC(n)h_\lambda^{(1)}(i\alpha r) \quad \begin{matrix} 1 & \text{even } \lambda \\ 1 & \text{odd } \lambda \end{matrix}$$

where

$$r = n\epsilon + 0.5(n - n_2 + |n - n_2|)\epsilon$$

Here j_λ is the spherical Bessel function and $h_\lambda^{(1)}$ is the spherical Hankel function of the first kind. These functions are provided by subroutine AJH. When the Coulomb kernel is being calculated, IZB computes

$$ZA1(n) = ZC(n)r^\lambda$$

$$ZA2(n) = ZC(n)r^{-\lambda-1}$$

Program IZC - Bound-State Kernel

The bound-state kernel is made up of a nuclear part and a Coulomb part. The nuclear part is calculated to be

$$B_N(n) = -4\pi V_0 \left(\frac{M_I}{M_C}\right)^3 \left[j_\lambda(i\alpha r) \int_r^\infty dr_1\, r_1^2 ZA2(n_1) + h_\lambda^{(1)}(i\alpha r) \int_0^r dr_1\, r_1^2 ZA1(n_1) \right]$$

where

$$r = n\epsilon + 0.5(n - n_2 + |n - n_2|)\epsilon$$

$$r_1 = n_1\epsilon + 0.5(n_1 - n_2 + |n_1 - n_2|)\epsilon$$

The Coulomb part is calculated to be

$$B_C(n) = \frac{B_S}{2\lambda + 1}\left(\frac{M_I}{M_C}\right)^3\left[r^{\lambda}\int_r^{R_O} dr_1 r_1^2 ZA2(n_1) + r^{-\lambda-1}\int_0^r dr_1\, r_1^2 ZA1(n_1)\right.$$

$$\left. - \delta_{\lambda O} f(r)\int_0^{R_O} dr_1\, r_1^2 ZA1(n_1)\right]$$

where $f(r)$ is as defined in the INTRODUCTION. When $L_I = 0$, B_N is provided by IZS, and when $L_I = 2$, B_N is provided by IZB. Otherwise B_N is calculated as shown previously. The quantity B_C is always calculated as shown previously. Finally, ZDEL = $B_N + B_C$ is the total bound-state kernel. If $B_S \neq 0$, the program points out the multipole moment

$$\frac{4\pi}{2\lambda + 1}\left(\frac{M_I}{M_C}\right)^3\int_0^{R_O} dr_1 r_1^2 \rho_{FI}^{\lambda}\left(\frac{M_I}{M_C} r_1\right) r_1^{\lambda}$$

where ρ_{FI}^{λ} is as defined in the INTRODUCTION.

Program 2VD - Kinetic Energy in Incident Channel

If $L_P = 1$, control is transferred to program 4, while if $L_P = 0$, the kinetic energy in the incident channel is evaluated by using subroutine TWO PD. The quantities evaluated are

$V(n) = \frac{\hat{\epsilon}^2}{6}\frac{ID}{\hbar^2} \times$ (real part of kinetic energy)

$W(n) = \frac{\hat{\epsilon}^2}{6}\frac{M_{ID}}{\hbar^2} \times$ (imaginary part of kinetic energy)

$VC(n) = \frac{\hat{\epsilon}^2}{6}\frac{M_{ID}}{\hbar^2} \times$ (kinetic energy for Coulomb scattering)

$\hat{\epsilon} = \epsilon_D \qquad n_2 > n$

$= 2\epsilon_D \qquad n > n_2$

Program 2VP - Kinetic Energy in Outgoing Channel

The kinetic energy in the outgoing channel is evaluated by using subroutine TWO PD. The quantities evaluated are

$$VA(n) = \frac{\hat{\epsilon}^2}{6}\frac{M_{FP}}{\hbar^2} \times \text{(real part of kinetic energy)}$$

$$WA(n) = \frac{\hat{\epsilon}^2}{6}\frac{M_{FP}}{\hbar^2} \times \text{(imaginary part of kinetic energy)}$$

$$VCA(n) = \frac{\hat{\epsilon}^2}{6}\frac{M_{FP}}{\hbar^2} \times \text{(kinetic energy for Coulomb scattering)}$$

$$\hat{\epsilon} = \epsilon_P \qquad n_2 > n$$

$$= 2\epsilon_P \qquad n_2 < n$$

Program 2XD - Radial Wave Function for the Incident Channel

By means of subroutine TWO AB the radial wave functions for the incident channel are calculated and are written on tape 4. These wave functions are represented here by

$$ZD(L,n) = XD(L,n) + iYD(L,n) = \chi^D_L(r)$$

where

$$r = n\epsilon_D + 0.5(n - n_2 + |n - n_2|)\epsilon_D$$

The radial wave functions for $L < L_{DD}$ are calculated by using $V(n) + iW(n)$ for the kinetic energy, while for $L_{CD} \geq L \geq L_{DD}$ the kinetic energy $VC(n)$ is used.

Program 2XP - Radial Wave Function for Outgoing Channel

By means of subroutine TWO AB the radial wave functions for the outgoing channel are calculated and are written on tape 3. These wave functions are represented here by

$$ZP(L,n) = XP(L,n) + iYP(L,n) = \chi^P_L(r)$$

where

$$r = n\epsilon_P + 0.5(n - n_2 + |n - n_2|)\epsilon_P$$

The radial wave functions for $L < L_{DP}$ are calculated by using VA(n) + iWA(n) for the kinetic energy, while for $L_{CP} \geq L \geq L_{DP}$ the kinetic energy VCA(n) is used.

Program 3B - Coulomb Scattering Amplitudes

Subroutine THREE B is used to calculate the Coulomb phase shifts $\sigma_D(L)$ for the incident channel and the Coulomb phase shifts $\sigma_P(L)$ for the outgoing channel.

Program 3A - Nuclear Scattering Amplitudes

Subroutine THREE A is used to calculate the scattering amplitudes and normalization factors for the radial wave functions. For a given radial wave function $\chi_L^A(A = D,P)$, the normalization factor C_L^A and the scattering amplitude A_L^A are determined by the requirement that

$$C_L^A \chi_L^A = -\frac{K_A R_O}{2}\left[y_L(K_A,R_O)^* + A_L^A y_L(K_A,R_O)\right]$$

where $y_L(K,r)$ is the Coulomb analog of the spherical Hankel function of the first kind. It is convenient to write

$$A_L^A = A_{NL}^A + \exp\left[i2\sigma_A(L)\right]$$

where A_{NL}^A is called the nuclear scattering amplitude and $\exp[i2\sigma_A(L)]$ is called the Coulomb scattering amplitude. For $L \geq L_{DA}$, A_{NL}^A is set equal to zero and C_L^A is set equal to $\exp[i\sigma_A(L)]$. To verify the validity of this step, the program prints out the real and the imaginary parts of $A^D_{N,L_{DD}-1}$ identified by DISTORTION CHECK D and the real and the imaginary parts of $A^P_{N,L_{DP}-1}$ identified by DISTORTION CHECK P. If $A^A_{N,L_{DA}-1}$ is not very small compared with 1, then L_{DA} should be increased by increasing W_1 or W_2.

Program 3A also calculates and prints out reduced widths for $r = R_2$ and $r = R_c$. The reduced width is taken to be

$$\text{reduced width} = \hbar^2[\text{ZDEL}(n)]^2/2M_{NC}r$$

where

$$r = n\epsilon_N + 0.5(n - n_2 + |n - n_2|)\epsilon_N$$

Program 4 - Radial Integrals

By means of subroutine FOUR the following radial integrals are evaluated:

$$S^O_{L,l} = \int_0^{R_O} dr\ Z(r')\chi^D_l(r'')\chi^P_l(r''')$$

$$S^C_{L,l} = \int_{R'}^{R_O} dr\ Z(r')\chi^D_l(r'')\chi^P_l(r''')$$

where

$$r = n\epsilon + 0.5(n - n_2 + |n - n_2|)\epsilon$$

$$Z(r') = ZDEL(n)$$

$$\chi^D_l(r'') = ZD(l,n)$$

$$\chi^P_L(r''') = ZP(L,n)$$

$$R'_C = M_C R_C / M_I \qquad I_R = 1,2$$

$$R'_C = M_I R_C / M_F \qquad I_R = 3,4$$

Program 5 - Coefficients of Legendre Polynomial Expansion

The coefficients of the Legendre polynomial expansion are calculated as

$$B^{\lambda\mu}_{LA} = V_I C^P_L \sum_l C^D_l S^A_{L,l} \Gamma^{\lambda\mu}_{Ll} (-1)^{(L+\lambda-l)/2} \qquad A = O,C$$

The quantities $\Gamma^{\lambda\mu}_{Ll}$ are provided by subroutine GAMMA.

Program 6 - Convergence Test and Total Cross Section

First, this program calculates and prints out the quantities

$$\frac{G_{L_{CP}}^{O}}{\sum_{O}^{L_{CP}} G_L^O} \quad \text{and} \quad \frac{G_{L_{CP}}^{C}}{\sum_{O}^{L_{CP}} G_L^C}$$

preceded by the words CONVERGENCE TEST. In the previous expressions,

$$G_L^A = \frac{4\pi}{2L+1} \sum_{\mu=-\lambda}^{\lambda} \left| B_{LA}^{\lambda\mu} \right|^2 (L + |\mu|)!/(L - |\mu|)! \qquad A = O, C$$

Next, the program prints out the words TOTAL CROSS SECTION followed by

$$R = 0 \qquad S = \eta \sum_{O}^{L_{CP}} G_L^O \qquad R = R_C \qquad S = \eta \sum_{O}^{L_{CP}} G_L^C$$

The quantities S are total direct-reaction cross sections according to the DWBA and the cutoff DWBA, respectively.

The convergence test is an indication of the error resulting from truncating the angular momentum expansion after $L_{CP} + 1$ terms. If the convergence test is not very small compared with 1, then L_{CP} should be increased by increasing W_4.

Program 7A - Direct-Reaction Amplitudes

Program 7A calculates the direct-reaction amplitudes as a function of center of mass angle. The amplitudes are given by

$$B_A^{\lambda\mu}(\theta) = \sum_{L=O}^{L_{CP}} B_{LA}^{\lambda\mu} P_L^{\mu}(\cos\theta) \qquad A = O, C$$

The associated Legendre polynomials P_L^{μ} are provided by subroutine LP. If $I_P = 0$, the amplitudes are printed out under the heading DIRECT-REACTION AMPLITUDES.

The real and the imaginary parts are identified as follows:

$$B_0^{\lambda\mu} = B1P + iB1M$$

$$B_C^{\lambda\mu} = B2P + iB2M$$

If $I_P > 0$ the transition amplitudes are punched on cards as well as being printed out, and if $I_P < 0$ the transition amplitudes are not read out at all.

Program 7B - Direct-Reaction Cross Section

The direct-reaction differential cross section is taken to be

$$\sigma_A(\theta) = \eta \sum_{\mu=-\lambda}^{\lambda} \left|B_A^{\lambda\mu}(\theta)\right|^2 \qquad A = 0, C$$

Program 7B calculates $\sigma_0(\theta)$ and $\sigma_C(\theta)$. The maximums of these two cross sections are determined and are printed out in the following statements:

NORMALIZATION FOR R = 0 IS

$\max[\sigma_0(\theta)]$ MB. PER STER.

NORMALIZATION FOR R = (R_C) IS

$\max[\sigma_C(\theta)]$ MB. PER STER.

NORMALIZATION FOR EXPT XSTN IS

$[\max(\sigma_{EX})]$ MB. PER STER.

The last statement appears only if the experimental cross sections are included in the input data.

Then the normalized cross section

$$\frac{\sigma_0(\theta)}{\max[\sigma_0(\theta)]} \qquad \frac{\sigma_C(\theta)}{\max[\sigma_C(\theta)]} \qquad \frac{\sigma_{EX}(\theta)}{\max[\sigma_{EX}(\theta)]}$$

and the momentum transfer

$$\sqrt{K_P^2 + K_D^2 - 2K_PK_D \cos\theta}$$

are printed out. The three normalized cross sections are also displayed on a

graphical plot.

Program 8 - Elastic Scattering Cross Sections

If $N_5 \neq 0$ the calculation ends with program 7. The differential cross section for elastic scattering is calculated for the incident channel and the outgoing channel by program 8 if $N_5 = 0$. The elastic cross section for the incident channel is

$$\sigma_D(\theta) = \left| (2iK_D)^{-1} \sum_L \left(A_L^D - 1 \right) P_L(\cos\theta) \right|^2$$

$$= \left| B^D + \sum_L (2iK)^{-1} A_{NL}^D P_L(\cos\theta) \right|^2$$

The Coulomb elastic cross section for the incident channel is

$$\sigma_{DC}(\theta) = |B^D|^2 = \left| (2iK_D)^{-1} \sum_L (2L+1) e^{i2\sigma_D(L)} P_L(\cos\theta) \right|^2$$

The Legendre polynomial P_L is provided by subroutine LP. The quantity B^D is the well known Coulomb scattering amplitude

$$B^D = \frac{-e^{i2\sigma_D(0)} \, \eta_D e^{-i\eta_D \ln \sin^2 \frac{\theta}{2}}}{2 \sin^2 \frac{\theta}{2}}$$

The program prints out $\sigma_D(\theta)$, $\sigma_{DC}(\theta)$, and $\sigma_D(\theta)/\sigma_{DC}(\theta)$. In a similar way the same quantities for the outgoing channel are calculated and are printed out. The calculation ends at this point.

Subroutine SZ - Surface Form Factor

Subroutine SZ calculates the function

$$AAT(n) = V_0 R_S [a_S (2 + X + X^{-1})]^{-1}$$

where

$$X = \exp[(r - R_S)/a_S]$$

$$r = n\epsilon + 0.5(n - n_2 + |n - n_2|)\epsilon$$

Subroutine AJH - Spherical Bessel or Hankel Function

Subroutine AJH calculates the spherical Bessel functions of imaginary argument $j_L(ix)$ or the spherical Hankel functions of the first kind of imaginary argument $h_L(ix)$. The first step of the calculation is the evaluation of

$$j_0(ix) = (e^x - e^{-x})(2x)^{-1}$$

$$ij_1(ix) = \left[(1 - x)e^x - (1 + x)e^{-x}(2x^2)^{-1}\right]$$

or

$$h_0(ix) = -e^{-x}(x)^{-1}$$

$$ih_1(ix) = -(1 + x)e^{-x}(x^2)^{-1}$$

Then the higher order functions are generated by the recursion relation

$$i^l z_l(ix) = \frac{2l - 1}{x} i^{l-1} z_{l-1}(ix) + i^{l-2} z_{l-2}(ix)$$

where

$z_l = j_l$ or h_l

AJH is also called upon to calculate x^l and x^{-l-1}.

Subroutine ONE Z - Bound-State Wave Function

Subroutine ONE Z calculates bound-state solutions of the Schroedinger equation for a particle moving in a potential well of the form $V(r) = V_C(r) - V_N F(r)$. The term $V_C(r)$ is the Coulomb potential due to a uniform sphere of charge:

$$V_C(r) = \frac{Z_N(Z_I - Z_N)e^2}{R_N} \begin{cases} \frac{3}{2} - \frac{1}{2}\left(\frac{r}{R_N}\right)^2 & r < R_N \\ \frac{R_N}{r} & r > R_N \end{cases}$$

For the form factor $F(r)$ there are the following three choices:

$$F(r) = \left\{1 + \exp\left[(r - R_N)/B_N\right]\right\}^{-1} \qquad N_D = 1$$

$$= \left\{\begin{array}{ll} 1 - \left(\frac{r}{B_N}\right)^2 & r < R_N \\ 0 & r > R_N \end{array}\right\} \qquad N_D = 2$$

$$= 1 - \left(\frac{r}{B_N}\right)^2 \qquad N_D = 3$$

There is also a spin-orbit term available when $N_D = 1$. This addition to $F(r)$ has the form

$$-\left[\frac{1}{2}\lambda_\pi^2 \overline{\sigma} \cdot \overline{l}\,\frac{1}{r}\frac{d}{dr}F(r)\right] C_S$$

where λ_π is the pion Compton wavelength.

The Schroedinger equation to be solved is

$$\left\{\frac{d^2}{dr^2} = \frac{2M_{IN}}{\hbar^2}\left[E_B + V(r)\right] - \frac{L(L+1)}{r^2}\right\}\chi_L^N = 0$$

where $L = \overline{l}$ or $\overline{l}'$. Near the origin, χ_L^N is represented by the series

$$\chi_L^N = r^{L+1}\sum_{n=0} C_n r^n$$

where

$$C_0 = [(2L+1)(2L-1)(2L-3)\ldots 3 \cdot 1]^{-1}$$

$$C_2 = -AC_0/(4L+6)$$

$$C_n = -(BC_{n-4} + AC_{n-2})/n(n+2L+1)$$

$$A = \frac{2M_{IN}}{\hbar^2}(V_N - E_B) - \frac{3K_N\eta_N}{R_N}$$

$$B = K_N \eta_N / R_N^3 \qquad N_D = 1$$

$$= \frac{K_N \eta}{R_N^3} - \frac{2M_{IN} V_N}{\hbar^2 B_N^2} \qquad N_D = 2,3$$

Near $r = R_O$, χ_L^N is represented by $e^{-K_N r}$. The solution is started from the values of χ_L^N given by the power series near the origin, and the values of χ_L^N at larger values of r are generated by the approximate recurrence relation

$$\chi_L^N(r + \delta) = \frac{[12 - 10\, q(r)]\chi_L^N(r) - q(r - \delta)\chi_L^N(r - \delta)}{q(r + \delta)}$$

In this way $\chi_L^N(r)$ is evaluated in the interval $0 < r < R_M$, where R_M is R_{N1} or R_{N2}. The symbol R_M is called the matching radius. The same recurrence relation is used to evaluate $\chi_L^N(r)$ in the interval $R_M < r < R_O$ by using $e^{-K_N r}$ to give starting values at $r = R_O$. The ratio of the wave functions at the two points R_M and $R_M + \delta$ is compared for the solution calculated for $r < R_M$ (inside) and for $r > R_M$ (outside). If the difference is not less than 10^{-N_3}, the value of V_N is changed and the calculation of wave function is repeated in the region where the potential is not negligible.

The first value of V_N used by the program is provided by the input data. If the input value of V_N is zero, an estimate of V_N will be provided by function subprogram VBEST. The value provided by VBEST will be the correct value of V_N if $N_D = 3$.

The number of nodes in the inside wave function is counted, and, if it does not match the bound-state radial quantum number, V_N is incremented by ± 2 DVN until the correct number of nodes is obtained. If the inside and the outside wave-function ratios fail to match, V_N is successively incremented until the difference in the inside and the outside wave-function ratio changes sign. Then subroutine INTRP is used to calculate a new value of V_N by interpolation from the previous two values of V_N. The value of χ_L^N is again calculated out from $r = 0$ and in from a radius beyond which the potential is less than 10^{-N_9} of its value at $r = R_M$ (for $N_D = 2$ or 3 only the inside wave-function calculation is repeated), and the inside and outside wave-function ratios are again compared at $r = R_M$. The process is repeated until the difference of the wave-function ratios falls below 10^{-N_3}.

When a function $\chi_L^N(r)$ is produced that has the correct number of nodes and

is smooth at $r = R_M$, the integral

$$I = \int_0^{R_0} dr \left[\chi_L^N(r)\right]^2$$

is evaluated. The bound-state wave function is then taken to be

$$Z(r) = I^{-1/2}\chi_L^N(r)r^{-1}$$

The calculated potential depths V_{N1} and V_{N2} are printed out. If $I_{WZ} \neq 0$, the initial and the final nuclear form factors, F_1 and F_2, and the initial and final wave functions, X_1 and X_2, will also be printed out.

Subroutine TWO PD - Kinetic Energy

Subroutine TWO PD calculates the kinetic energy to be used in the calculation of the continuum radial wave functions carried out by subroutine TWO AB. The quantities evaluated for the incident channel calculation are

$$\left.\begin{aligned} V(n) &= \frac{\hat{\epsilon}^2}{12}\left(K_D^2 - \frac{2\eta_D K_D}{r}\right) \\ W(n) &= 0 \\ VC(n) &= \frac{\hat{\epsilon}^2}{12}\left(K_D^2 - \frac{2\eta_D K_D}{r}\right) \end{aligned}\right\} S_D < r < R_0$$

$$\left.\begin{aligned} V(n) &= \frac{\hat{\epsilon}^2}{12}\left[K_D^2 - \frac{2\eta_D K_D}{r} - \frac{2M_{ID}}{\hbar^2} V_D f(r)\right] \\ W(n) &= -\frac{\hat{\epsilon}^2}{12}\frac{2M_{ID}}{\hbar^2}\left[W_D f(r) + X_D g(r)\right] \\ VC(n) &= \frac{\hat{\epsilon}^2}{12}\left(K_D^2 - \frac{2\eta_D K_D}{r}\right) \end{aligned}\right\} \bar{R}_D < r < S_D$$

$$\left.\begin{aligned} V(n) &= \frac{\hat{\epsilon}^2}{12} K_D^2 - \eta_D K_D \left(\frac{3}{\bar{R}_D} - \frac{r^2}{\bar{R}_D^3}\right) - \frac{2M_{ID}}{\hbar^2} V_D f(r) \\ W(n) &= -\frac{\hat{\epsilon}^2}{12} \frac{2M_{ID}}{\hbar^2} \left[W_D f(r) + X_D g(r)\right] \\ VC(n) &= \frac{\hat{\epsilon}^2}{12} \left(K^2 - \frac{2\eta_D K_D}{r}\right) \end{aligned}\right\} 0 < r < \bar{R}_D$$

where

$$r = n\epsilon_D + 0.5(n - n_2 + |n - n_2|)\epsilon_D$$

$$\hat{\epsilon} = \epsilon_D \qquad n \leq n_2$$

$$= 2\epsilon_D \qquad n > n_2$$

$$f(r) = P\left[1 + \exp\left(\frac{r - \bar{R}_D}{a_D}\right)\right]^{-1} \qquad r > \rho_D$$

$$= P \qquad r > \rho_D$$

$$g(r) = P \frac{XR_D}{Xa_D}\left[2 + \exp\left(\frac{r - XR_D}{Xa_D}\right) + \exp\left(\frac{XR_D - r}{Xa_D}\right)\right]^{-1}$$

The corresponding expressions for the outgoing channel result when the subscripts I and D that appear in the previous equations are replaced by F and P, and when V, W, and VC are replaced by VA, WA, and VCA.

Subroutine TWO AB - Radial Wave Function

Subroutine TWO AB calculates the radial wave functions for the incident and the outgoing channels. The expressions appropriate to the incident channel will be given. The radial wave functions are solutions to

$$\left[\frac{d^2}{dr^2} + \frac{12}{\hat{\epsilon}^2}(V + iW) - \frac{L(L+1)}{r^2}\right]\chi_L^D = 0$$

For $L \geq L_{DD}$, these solutions are approximated by the Coulomb radial wave func-

tions that are solutions to

$$\frac{d^2}{dr^2} + \frac{12}{\hat{\epsilon}^2} VC - \frac{L(L+1)}{r^2} \chi_L^D = 0$$

The quantities V, W, and VC are the kinetic energies provided by program 2VD. Also,

$$\hat{\epsilon} = \epsilon_D \qquad n \leq n_2$$

$$= 2\epsilon_D \qquad n > n_2$$

$$r = n\epsilon_D + 0.5(n - n_2 + |n - n_2|)\epsilon_D$$

In the interval $0 < r < N_0 L\epsilon_D$, a power series is used to represent χ_L^D:

$$\chi_L^D = C_{LD} r^{L+1} \sum_{\alpha=0} \varphi_\alpha r^\alpha$$

where

$$C_{LD} = \frac{\sqrt{L^2 + \eta_D^2}}{L(2L+1)} C_{L-1D}$$

For $L < L_{DD}$,

$$\varphi_0 = 1 \qquad \varphi_1 = 0$$

$$\varphi_\alpha = -[\alpha(\alpha + 2L + 1)]^{-1}(\lambda_0 \varphi_{\alpha-2} + \lambda_2 \varphi_{\alpha-4})$$

$$\lambda_0 = K_D^2 - 3K_D\eta_D\bar{R}_D^{-1} - \frac{2M_{ID}}{\hbar^2}(V_D + iW_D)f(r) - \frac{2M_{ID}}{\hbar^2} iX_D g(r)$$

$$\lambda_2 = K_D\eta_D\bar{R}_D^{-3}$$

For $L \geq L_{DD}$,

$$\varphi_0 = 1 \qquad \varphi_1 = \eta_D K_D (L+1)^{-1}$$

$$\varphi_\alpha = -[\alpha(\alpha + 2L + 1)]^{-1}\left(K_D^2\varphi_{\alpha-2} - 2K_D\eta_D\varphi_{\alpha-1}\right)$$

Only the first three terms of the power series are used, except at the last two points of the interval where N terms are taken. For $L < L_{DD}$, N is the smallest integer for which

$$10^{-N_6} > \frac{r^N(|\mathrm{Re}\varphi_N| + |\mathrm{Im}\varphi_N|)}{\left|\mathrm{Re}\sum_0^N \varphi_\alpha r^\alpha\right| + \left|\mathrm{Im}\sum_0^N \varphi_\alpha r^\alpha\right|}$$

For $L \geq L_{DD}$, N is the smallest integer for which

$$10^{-N_6} > \frac{r^N|\varphi_N| + r^{N-1}|\varphi_{N-1}|}{\left|\sum_0^N \varphi_\alpha r^\alpha\right|}$$

Using the two accurate values of χ_L^D at $r \approx N_0 L\epsilon_D$ the program proceeds to use the following scheme to calculate subsequent values of χ_L^D:

$$\chi_L^D(r + \delta) = \frac{[12 - 10\, q(r)]\chi_L^D(r) - q(r - \delta)\chi_L^D(r - \delta)}{q(r + \delta)}$$

where

$$q(r) = 1 - \frac{\delta^2}{12}\frac{L(L + 1)}{r} - \frac{\delta^2}{\hat{\epsilon}^2}(V + iW)$$

This scheme is based on the Taylor's series expansion of χ_L^D at r. The lowest order term neglected to get the previous formula is

$$\delta^6[240\, q(r + \delta)]^{-1}\frac{d^6}{dr^6}\chi_L^D(r)$$

This scheme is begun at $r \approx N_0 L\epsilon_D$ rather than at the origin in order to avoid the point where $q(r)$ vanishes. At this point round-off errors seriously affect the accuracy of the scheme. For this reason N_0 should be greater than 1/3. The value $N_0 = 1$ has been found to serve well. Choosing N_0 too large will impair the accuracy of the power series.

Subroutine THREE B - Coulomb Scattering Amplitudes

Subroutine THREE B calculates the Coulomb phase shifts $\sigma_A(L)$, $A = D, P$.

The Coulomb phase shift is defined by

$$\sigma_A(L) = \arg \Gamma(L + 1 + i\eta_A)$$

For sufficiently high values of L, Stirling's approximation can be used to evaluate the Γ-function. Thus,

$$\sigma_A(L) \approx (L + 0.5)\beta + \eta_A \ln \alpha - \eta_A - \frac{\sin \beta}{12\alpha}$$

$$+ \frac{\sin 3\beta}{360\ \alpha^3} - \frac{\sin 5\beta}{1260\ \alpha^5} + \frac{\sin 7\beta}{1680\ \alpha^7} - 0.00084175\ \frac{\sin 9\beta}{\alpha^9} + \ldots$$

where

$$\beta = \tan^{-1}[\eta/(L + 1)]$$

$$\alpha = \left[(L + 1)^2 + \eta_A^2\right]^{1/2}$$

The previous expression is used to evaluate $\sigma_A(50)$. Then the Coulomb phase shifts for lower L are generated by the recurrence relation

$$\sigma_A(L - 1) = \sigma_A(L) - \tan^{-1}(\eta_A/L)$$

Subroutine THREE A - Nuclear Scattering Amplitudes

Subroutine THREE A first calculates $y_L(K_A, r)$ at $r = R_0^A = n_2\epsilon_A + (n_0 - n_2)2\epsilon_A$ and at $r = R_0^A - 2\epsilon_A$, where A = D, P. The function $y_L(K_A, r)$ is the Coulomb analog of the spherical Hankel function of the first kind. The following asymptotic expansion is used to evaluate y_L:

$$y_L(K_A, r) \cong \frac{e^{i\theta}}{iK_A r} \sum_{n=0} p_n$$

where

$$p_0 = 1$$

$$p_n = \frac{(i\eta_A - L - 1 + n)(i\eta_A + L + n)p_{n-1}}{n(2iK_A r)}$$

The series is terminated after $N + 1$ terms, where N is the smallest integer for which

$$10^{-N_2} > \frac{|\mathrm{Re}\ p_N|}{|\mathrm{Re} \sum_0^N p_n| + |\mathrm{Im} \sum_0^N p_n|}$$

and

$$10^{-N_2} > \frac{|\mathrm{Im} p_N|}{|\mathrm{Re} \sum_0^N p_n| + |\mathrm{Im} \sum_0^N p_n|}$$

or $N = N_{10}$. If $N = N_{10}$, a statement that the asymptotic series has failed to converge is printed out.

The normalization factor C_L^A and the scattering amplitude A_L^A are determined from the equations

$$C_L^A X_0 + A_L^A Y_0 = -Y_0^*$$

$$C_L^A X_1 + A_L^A Y_1 = -Y_1^*$$

where

$$X_0 = \chi_L^A(R_0^A) \qquad X_1 = \chi_L^A(R_0^A - 2\epsilon_A)$$

$$Y_0 = \frac{K_A R_0^A}{2} y_L(K_A, R_0^A) \qquad Y_1 = \frac{K_A(R_0^A - 2\epsilon_A)}{2} y_L(K_A, R_0^A - 2\epsilon_A)$$

Thus,

$$C_L^A = \frac{Y_1^* Y_0 - Y_0^* Y_1}{X_0 Y_1 - X_1 Y_0}$$

$$A_L^A = \frac{Y_1^* X_0 - Y_0^* X_1}{X_1 Y_0 - X_0 Y_1}$$

The nuclear scattering amplitude is then taken to be

$$A_{NL}^A = A_L^A - \exp[i2\sigma_A(L)]$$

Subroutine FOUR - Radial Integral

Program 4 multiplies together the bound-state kernel Z and the outgoing channel radial wave function χ_L^P. Subroutine FOUR then multiplies the incident channel wave function χ_l^D by the product $Z\chi_L^P$ to form

$$F(n) = Z(r_N)\chi_L^P(r_P)\chi_l^D(r_D)$$

where

$$r_M = n\epsilon_M + 0.5(n - n_2 + |n - n_2|)\epsilon_M$$

$M = N, P, D$

The following sum is then evaluated:

$$S_{L,l}^0 = \frac{\epsilon}{2} F(1) + \frac{3\epsilon}{8} [F(1) + 3F(2) + 3F(3) + 2F(4) + 3F(5) + 3F(6)$$

$$+ 2F(7) + \ldots + 3F(n_2 - 2) + 3F(n_2 - 1) + F(n_2)]$$

$$+ \frac{3}{4} \epsilon[F(n_2) + 3F(n_2 + 1) + 3F(n_2 + 2) + 2F(n_2 + 3) + \ldots$$

$$+ 3F(n_0 - 1) + 2F(n_0)]$$

This sum represents the integral

$$S_{L,l} \approx \int_0^{R_0} dr\ Z(r_N)\chi_L^P(r_P)\chi_l^D(r_D)$$

where

$$r = n\epsilon + 0.5(n - n_2 + |n - n_2|)\epsilon$$

$$R_0 = n_2\epsilon + (n_0 - n_2)2\epsilon$$

It is based on the 3/8's rule

$$\int_A^B dr\ F(r) \approx \frac{3}{8} \delta[F(a) + 3F(A + \delta) + 3F(A + 2\delta)$$

$$+ 2F(A + 3\delta) + \ldots + 3F(B - \delta) + F(B)]$$

Subroutine FOUR uses a similar procedure to evaluate the integral

$$S^{C}_{L,l} = \int_{R'_C}^{R_O} dr\ Z(r_N)\chi^{P}_{L}(r_P)\chi^{D}_{l}(r_D)$$

where

$$R'_C = n_C\epsilon + 0.5(n_C - n_2 + |n_C - n_2|)\epsilon$$

Subroutine LP - Associated Legendre Polynomials

The associated Legendre polynomial $P^{M}_{L}(x)$ is generated from $P^{M}_{M}(x)$ and $P^{M}_{M+1}(x)$ by the recursion relation

$$P^{M}_{L}(x) = \frac{(2L - 1)xP^{M}_{L-1} - (L - 1 + M)P^{M}_{L-2}}{L - M}$$

The equations used for P^{M}_{M} and P^{M}_{M+1} are

$$P^{M}_{M}(x) = \frac{(2M)!2^{-M}(1 - x^2)^{M/2}}{M!}$$

and

$$P^{M}_{M+1}(x) = (2M + 1)xP^{M}_{M}(x)$$

Subroutine GAMMA - The Gamma Coefficient

The gamma coefficient is defined by

$$\Gamma^{lm}_{L\lambda} = \frac{(2L + 1)(2\lambda + 1)}{2l + 1}(L\lambda 00|L\lambda l0)(L\lambda m0|L\lambda lm)\left[\frac{(L - |m|)!}{(L + |m|)!}\right]^{1/2}$$

Substituting explicit expressions for the vector addition coefficients gives

$$\Gamma^{l m}_{L\lambda} = (-1)^{G+L}(2L+1)(2\lambda+1)\frac{l!(l-|m|)!}{(2l+1)!}\left[\frac{\binom{l+|m|}{|m|}}{\binom{l}{|m|}}\right]^{1/2}$$

$$\times \frac{\binom{L-|m|}{l-|m|}\binom{l}{G-L}\binom{G}{L}}{\binom{2G+1}{2l+1}} \sum_{t} \frac{(-1)^t \binom{2G-2L}{t}\binom{2G-2\lambda}{l-m-t}\binom{\lambda}{t}}{\binom{L-l+t}{t}}$$

where

$$G = \frac{1}{2}(L+\lambda+l)$$

$$\binom{a}{b} = \frac{a!}{(a-b)!b!}$$

The previous expression is used to evaluate the gamma coefficient, and use is made of function subprogram FCTRL.

Subroutine PLOT - Plot Graph

Subroutine PLOT uses subroutine PLOTMY to produce a graphical print-out of the calculated direct-reaction cross sections together with the experimental cross section included in the input data. If $Y_L = 0$, the cross section will be plotted, while $Y_L = 1$ will cause the logarithm of the cross section to be plotted. Before being plotted, the cross sections are normalized so that the maximum values are 1. The vertical scale of the plot will be $Y_S/20$ to one line space if $Y_L = 1$, and it will be $Y_S/100$ if $Y_L = 0$. It has been found that $Y_S = 2$ is a convenient choice for most cases. The information entered on input card 22 is used as a heading to identify the plot.

Function Subprogram FCTRL - Factorial Function

Subprogram FCTRL evaluates the function

$$\text{FCTRL}(J_N, D_N, N_N, J_D, D_D, N_D, J) = \frac{Z_1^N Z_2^N \cdots Z_{N_N}^N}{Z_1^D Z_2^D \cdots Z_{N_D}^D}$$

where

$$Z_M^N = J_N(M)[J_N(M) - D_N][J_N(M) - 2D_N] \ . \ . \ . \ [J_N(M) - JD_N]$$

and

$$Z_M^D = J_D(M)[J_D(M) - D_D][J_D(M) - 2D_D] \ . \ . \ . \ [J_D(M) - JD_D]$$

The J_N that appears in the argument of FCTRL represents an array of N_N numbers: $J_N(1)$, $J_N(2)$, . . ., and $J_N(N_N)$. Similarly, J_D represents an array of N_D numbers: $J_D(1)$, $J_D(2)$, . . ., and $J_D(N_D)$. The numbers N_N and N_D must be no greater than 10. The factorial function subprogram is used by subroutine GAMMA.

Function Subprogram VBEST - Bound-State Potential Depth

The function subprogram VBEST calculates the exact depth V_N of the harmonic oscillator potential. This calculation is based on the following considerations. The Schroedinger equation for the bound particle is

$$\left\{\frac{d^2}{dr^2} + \frac{2M_{IN}}{\hbar^2} V_N\left[1 - \left(\frac{r}{B_N}\right)^2\right] - \frac{2M_{IN}}{\hbar^2} E_B - \frac{L(L+1)}{r^2}\right\} \chi_L^N = 0$$

which can be rewritten to read

$$\left[\frac{d^2}{dr^2} - \frac{m^2\omega^2r^2}{\hbar^2} + \hbar\omega\left(2n + L - \frac{1}{2}\right)\frac{2m}{\hbar^2} - \frac{L(L+1)}{r^2}\right]\chi_L^N = 0$$

where $n = 1, 2, \ . \ . \ .$ Thus, it can be required that

$$m = M_{IN}$$

The first approximation is given by

$$x_3 = \frac{f(x_1)x_2 - f(x_2)x_1}{f(x_1) - f(x_2)}$$

and the second approximation is given by

$$x_4 = \frac{B \pm \sqrt{B^2 - 4AC}}{2A}$$

where

$$A = \sum_{i=1}^{3} C_i$$

$$B = \sum_{i=1}^{3} C_i(x_j + x_k) \qquad i,j,k \text{ cyclic}$$

$$C = \sum_{i=1}^{3} C_i x_j x_k \qquad i,j,k \text{ cyclic}$$

$$C_i = f(x_i)(x_j - x_k) \qquad i,j,k \text{ cyclic}$$

If $f(x)$ were a straight line, $A = 0$, $B = 0$, and x_4 would be indeterminate. For an arbitrary regular function $f(x)$, if an attempt were made to fit a parabola through three points very near the exact root, the quantities A and B would be very close to zero. Thus, parabolic interpolation cannot be used after a certain degree of accuracy has been attained.

$$\hbar\omega\left(2n + L - \frac{1}{2}\right) = V_N - E_B$$

$$\omega^2 = \frac{2V_N}{M_{IN}B_N^2}$$

From the last two equations

$$V_N = \left(A + \sqrt{A^2 + E_B}\right)^2$$

where

$$A = \frac{2n + L - \frac{1}{2}}{B_N}\sqrt{\frac{\hbar^2}{2M_{IN}}}$$

The value of V_N is calculated from the previous expression. For Saxon wells the value $V_N = 55$ Mev is used.

Subroutine INTRP - Interpolation

The subroutine INTRP is designed to solve for the roots of a function $f(x)$. Points on the curve $f(x)$ against x are to be computed at intervals by the calling program until a zero is passed. Suppose the points x_1, $f(x_1)$ and x_2, $f(x_2)$ straddle the zero. This information is placed at the disposal of

INTRP by two successive statements. INTRP then calculates a straight line joining these points. The zero of the line, denoted by x_3, is taken to be the first approximation to the root. The calling program then calculates $f(x_3)$. Control is then returned to INTRP, which fits a parabola to points 1, 2, and 3. The zero of the parabola nearest x_3 is taken to be the second approximation x_4.

Subroutine INTRP computes successive approximations x_n to the root of $f(x)$ by parabolic interpolation until the quantity A is 10^{-4} of its original value. INTRP then switches back to linear interpolation. The search for improved approximations continues until the calling program is satisfied with the accuracy of the result.

Lewis Research Center
National Aeronautics and Space Administration.
Cleveland, Ohio, November 29, 1963

REFERENCE

1. Tobocman, W.: Theory of Direct Nuclear Reactions. Oxford Univ. Press, 1961.